Room-temperature Compressibilities of MnO and CdO: A Further Examination of Effects of Different Cation Type On The Bulk Modulus Systematics	X17B1

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MnO manganosite and CdO monteponite, representatives of the 3d and 4d transition metal monoxides, both have a cubic structure of the rock-salt type (i.e., B1 structure) at 1 atm up to their melting temperatures. CdO does not undergo any structure change up to pressures of 30 GPa whereas MnO may transform to a phase that is possibly tetragonal near 10 GPa (Drickmer et al. 1966). In the absence of crystal-field stabilization, resulted from the valence electron configuration of Mn^{+2} (i.e., $3d^5 4s^2$), MnO represents an ideal compound among 3d transition metal monoxides to be compared with CdO for exploring effects of different cation type on crystal compressibility. In this work, pressure-volume measurements were carried out at room temperature with energy-dispersive synchrotron X-ray diffraction. The two oxide samples were studied in the same experiment for direct comparison.

Room-temperature volume measurements up to 8.1 GPa revealed that MnO and CdO have identical compressibility in the pressure range studied. In the plot of bulk modulus vs. unit-cell volume, CdO plots more than 20 GPa above the trend of 3d transition metal monoxides, resulting in significant deviation from empirical predictions of constant K_0V_0. The present observations are in favor of our earlier suggestion (Zhang and Reeder, 1998) that, for isostructural solids, the empirically predicted bulk modulus-volume relationship may be limited to their subsets that share the same valence electron character (i.e., s-type vs. 3d vs. 4d). For cations forming transition metal monoxides, variations of Pauling electronegativity with ionic radius show differences that are qualitatively similar to the observed trends of bulk modulus, suggesting that bond covalency differences may contribute to the different behaviors between the 3d and 4d transition metal monoxides.

References

Drickamer, H.G., Lynch R.W., Clendenen R.L. and Perez-Albuerne E.A. (1966) X-ray diffraction studies of the lattice parameters of solids under very high pressure. Solid State Physics, 19, 135-229.

Zhang, J. and Reeder R.J. (1998) Comparative compressibilities of calcite-structure carbonates: Deviations from empirical predictions. American Mineralogist, in press.